OCO (Orbiting Carbon Observatory) -2

ABSCO User Guide

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Revision History

Revision Date	Changes	Author
3 December 2013	Initial Release of “Spectroscopic Needs for OCO-2”	V. Payne
4 March 2016	Updated for ABSCO v5.0, now named “ABSCO User Guide”	V. Payne
14 March 2017	Updated CO2 scaling recommendation for SCO2 and updated references	V. Payne
24 July 2017	Updated to indicate that ABSCO v5.0 utilized in version 8 Level 2 algorithm	V. Payne

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1 Introduction

1.1 Scope and Background

This document is intended to provide an overview of the v5.0 ACOS/OCO-2 absorption coefficient (ABSCO) tables, key features and issues and potential directions for future research.

The ACOS/OCO-2 ABSCO tables are "lookup tables" that supply cross section values for absorbing gases in the Level 2 algorithm (L2) retrieval process. They record molecular absorption cross-sections over the range of relevant wavelengths, temperatures, and pressures in units of cm^2/mol for the gases O_2, H_2O, and CO_2. During the L2 generation process the retrieval algorithm computes atmospheric absorption at each relevant temperature, pressure, and wavelength using linear interpolation. Successive versions have refined these tables by incorporating new laboratory results and theoretical models for increasingly accurate absorption coefficients. ABSCO tables are released together with each major build of the OCO-2 Level 2 algorithm. ABSCO v5.0 tables used within version 8 of the OCO-2 Level 2 retrievals.

The tables can be computed at a spectral resolution of 0.002 cm^{-1} (required for validation of the tables using high resolution laboratory spectra) but the current L2 retrieval code uses a spectral resolution of 0.01 cm^{-1}.

1.2 Document Overview

Section 2 describes the absorption cross-section computation, while Section 3 describes the format of the ABSCO HDF files.

1.3 Data Usage Policy

The OCO-2 ABSCO tables are provided freely to the public, on request. We request that when publishing using the tables, please acknowledge NASA and the ACOS/OCO-2 project.

- Include OCO-2 as a keyword to facilitate subsequent searches of bibliographic databases if it is a significant part of the publication
- Include a bibliographic citation for the tables. The most relevant citations currently are Drouin et al. (2017) for the O2 A-band, Benner et al. (2016) for the 2.06 μm strong CO2 band and Devi et al. (2016) for the 1.6 μm weak CO2 band.
- We recommend sending courtesy copies of publications to the OCO-2 Project Scientist, Michael.R.Gunson@jpl.nasa.gov.

2 Absorption cross section computation

This section describes the studies providing line parameters for each of the main absorbing gases. Due to the modular nature of the ABSCO calculation, different bands rely on different codebases to compute the absorption cross sections. In summary, the LABFIT codebase from Benner (2011) provides CO_2 cross sections. For ABSCO v5.0, we implement databases from Drouin et

al. (2017), Benner et al. (2016) and Devi et al. (2016) for the O_2 A-band and the 2.06 μm and 1.6 μm CO_2 bands, respectively. The procedure and modeling assumptions for the ABSCO calculation are detailed at greater length in Thompson et al. (2012).
In v5.0, the table format is a four-dimensional array to accommodate an additional "foreign broadener gas" dimension. This allows cross sections to be parameterized by temperature, pressure, and the volume mixing ratio of one other atmospheric gas. All tables are provided in this 4D format, though the calculations only incorporate broadening by H_2O of O_2 and CO_2. CH_4 tables using the HITRAN line list are now also available; they are computed over both CO_2 spectral windows. The temperature range has 17 levels and is intended to cover extremely low (terrestrial) temperatures. Table 1 below gives more detailed information on several key parameter sources.

2.1 Scaling of absorption cross-sections

The ABSCO v5.0 tables are used in the version 8 OCO-2 Level 2 algorithm. The scaling information provided here is based on recommendations from the ABSCO team.

No scaling factors are applied to the ABSCO O2 tables. Tests using ground-based FTS spectra indicate that the Drouin et al. (2017) parameters result in retrieved surface pressure values that are in good agreement with ground truth. Initial tests using selected OCO-2 test datasets also indicate no need for scaling.

In the 1.6 μm (weak) CO2 band, tables calculated using the Devi et al. (2016) database are scaled by a constant factor of 1.014. This number represents a ratio between line intensities in the Devi et al. (2016) database and reference intensity measurements from our NIST ABSCO team members, described in Polyansky et al. (2015). In tests using single-band XCO2 retrievals from ground-based FTS spectra, we find that application of this constant scaling results in improved agreement between our single-band retrievals and the XCO2 values reported by the Total Column Carbon Observing Network (TCCON). For the 1.6 μm band, this scaling factor is already factored into the ABSCO v5.0 tables. The user should not scale the 1.6 μm tables.

In the 2.06 μm (strong) CO_2 band, the ABSCO tables are calculated using the Benner et al. (2016) database. We recommend that the users should scale the ABSCO tables by a factor of 1.004 in this band. We do not yet have "reference" intensity measurements for this band. We do have new ab initio intensity calculations from Jonathon Tennyson's group, described in Zak et al. (2016). In the weak CO2 band, the Tennyson calculations agreed very well with the NIST reference measured intensities. The ratio between the strong 2.06 μm lines in Zak et al. and Benner et al. (2016) is 1.006. In tests using single band retrievals from ground-based FTS spectra, the inferred scaling needed for agreement with TCCON XCO2 values is subject to scatter and to airmass dependence, but we find that an approximate scaling of 1.006 +/- 0.004 would be appropriate at low airmass. In tests within the OCO-2 Level 2 algorithm, using OCO-2

radiances, we find that a scaling of 1.004 for the 2.06 μm ABSCO table provides the best agreement between single-band retrievals performed using this band compared with single-band retrievals performed using the 1.6 μm ABSCO table as described above.

Table 1: ABSCO v5.0 Parameter Sources

	0.76μm O_2	1.61μm CO_2	2.06μm CO_2	H_2O
Spectral range	12745-13245 cm^{-1}	4700-6500cm^{-1}	4700-6500cm^{-1}	12745-13245cm^{-1} 4700-6500cm^{-1}
Spectral resolution	0.01cm^{-1} or 0.002cm^{-1}	0.01 cm^{-1} or 0.002cm^{-1}	0.01 cm^{-1} or 0.002cm^{-1}	0.01 cm^{-1} or 0.002cm^{-1}
Line parameters	Drouin (2017)	Devi (2016b)	Devi (2016a)	Rothman (2013), Rothman (2010)
ABSCO scaling	None	Included in tables, Based on Polyansky (2015)	To be applied by user, Based on Zak (2015)	None
Continuum	Drouin (2016)	-	Thompson et al. (2012)	Mlawer (2012) *

*see text for further details

0.76um O_2 Detail

Spectral line parameters, line mixing and collision-induced absorption for O2 are described in Drouin et al. (2017).

Parameters for broadening of O_2 by H_2O come from the study by Drouin et al. (2014).

1.6μm and 2μm CO_2 Detail

The CO_2 bands use line parameters and mixing models derived from studies by Devi et al. (2016) and Benner et al. (2016). The computation incorporates a speed dependent line profile with tridiagonal line mixing. The parameters are derived from fits to laboratory spectra at multiple temperatures. Parameters for foreign broadening of CO_2 by H_2O come from studies by Sung et al (2009). This study treated the 4.3μm band only. However, it is likely that these can be safely extrapolated to the other bands as well, and we favor this approach until additional direct laboratory data is available.

We note one important difference between the reference databases and our computed absorption coefficients. We found it necessary to incorporate an additional continuum absorption in the 2.06 um CO_2 band which takes the shape of two Gaussian distributions centered at 4853.5 and 4789 wavenumbers, with respective standard deviations of 10 and 8 wavenumbers and intensity scalings of 2.1e-24 and 4.2e-25, respectively (this is the intensity at 1 Atm, but absorption at

other levels scales in proportion to pressure). These parameters were set to minimize error in retrievals with TCCON uplooking FTS spectra.

H_2O Detail

We incorporate H_2O line parameters from the HITRAN 2012 compilation. We compute the H_2O Continuum using the AER MT_CKD codes (Mlawer et al., 2012). 1.6μm parameters are from HITRAN 2008, with the exception of a single line near 6290cm^{-1} that we modified empirically by hand. This procedure, performed with the help of Dr. Iouli Gordon, reduced a prominent residual that we noted in both TCCON and GOSAT atmospheric retrievals. New line parameters from the HITEMP database (Rothman et al. 2010) have been used for weak water lines in the Oxygen A Band. We use an unofficial modified version of the AER MT_CKD continuum (Mlawer et al. 2012), supplied for testing purposes only by Eli Mlawer. This increases the continuum slightly over the previous version of the AER MT_CKD model in the OCO-2 spectral intervals. This revision offers a conservative compromise between the previous continuum and new measurements by Ptashnik et al. (2011). The revised MT_CKD also falls relatively close to new measurements by Mondelain et al. (2013).

3 HDF5 Format Specification

The ABSCO tables are provided in an HDF5 format. The table is a 4D structure indexed in the following order:

- pressure levels 1 to N_{pres}
- temperature levels from 1 to N_{temps}
- foreign broadener vmrs from 1 to N_{vmrs}
- frequencies from 1 to N_{freqs}

In general, each table models one absorbing gas and up to one foreign broadening gas (here, always H_2O). We refer to the abosrber's HITRAN gas index value with the symbol Q_{abs} and its HITRAN isotope index as R_{abs}. The foreign broadener index is $Q_{brd.}$

The HDF file is has the following format:

– **File:** The top-level file object represents a collection of one or more absorber gas cross sections that have been computed for a common spectral range and set of atmospheric conditions. The file contains top-level attributes:
  - version: a version string describing the table release
  - addl_ident: a special identifier string, if any
  - gas_name: a string such as "o2"
  - wn_begin: the starting wavenumber
  - wn_end: the ending wavenumber
  - comment: a space for notes about the table creation
- **Gas_[Q_{abs}]_Absorption** The absorption coefficients are a 4D table of size N_{pres} x N_{temps} x N_{vmrs} x N_{freqs} and are indexed in that order. The dataset attributes are:
  - addl_ident: a special identifier string, if any
  - gas_name: a string such as "o2", which should match its filename
  - comment: a space for notes

- **Gas_Index** a string containing the 2 digit HITRAN index of the principal absorbing gas, equivalent to Q_{abs} above.
- **Pressure** The pressure is a dataset of size N_{pres} representing the pressure in Pascals at each atmospheric level in the table
- **Temperature** Temperature is a 2D dataset of degrees Kelvin, of shape N_{pres} x N_{temps} It records the temperature grid point values, which might differ depending on pressure level.
- **Broadener_[Q_{brd}]_VMR** A dataset of size N_{vmrs} representing the different volume mixing ratios at which the foreign broadening gas is modeled. Q_{brd} is a HITRAN index. Now we only model H_2O broadening, so the index is always 01.
    - broadener_name: the string "h2o"
- **Broadener_Index** a string contraining the 2 digit HITRAN index of the broadening gas, equivalent to Q_{brd} above
- **Wavenumber** The Wavenumber object is a dataset of size N_{freqs} describing the frequency grid spacing.

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